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Universal adiabatic dynamics in the vicinity of a quantum critical point

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We study temporal behavior of a quantum system under a slow external perturbation, which drives the system across a second-order quantum phase transition. It is shown that despite the conventional adiabaticity conditions are always violated near the critical point, the number of created excitations still goes to zero in the limit of infinitesimally slow variation of the tuning parameter. It scales with the adiabaticity parameter as a power related to the critical exponents z and ν characterizing the phase transition. We support general arguments by direct calculations for the Boson Hubbard and the transverse field Ising models.

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Quantum phase transitions have attracted a lot of theoretical and experimental attention in recent decades, see for example Ref. 1. They are driven entirely by quantum fluctuations and occur at zero temperature. In this paper, we will be interested in second-order transitions, which are characterized by universal properties near the critical point. Usually these properties can be revealed experimentally by measuring various correlation functions. Since the relaxation time in most of conventional condensed matter systems is relatively short, only equilibrium or steady-state regimes are experimentally relevant. On the other hand recent progress in the realization of ultracold atomic gases[2] made it possible to study experimentally both equilibrium and strongly out of equilibrium properties of the interacting quantum systems. Thus observation of the superfluid-to-insulator transition[3] relied on the reversibility of the phase coherence after the system was slowly driven to the insulating state and then back. In the same experiment, another resonant feature was observed if the Mott insulator is a subject to an external linear potential of a particular strength. This feature was later interpreted later as an Ising-type quantum phase transition between normal and dipolar states.[4] The other big advantage of atomic systems is that the parameters governing the transition can be tuned continuously during a single experiment, so that, for example, it is possible to cross a quantum critical point in a real time.

Let us consider now a specific situation, where some system was initially in the ground state. Then a tuning parameter was slowly changed to drive it through a critical point. From general principles, we know that the system should remain in the ground state as long as it is protected by the gap from the excitations. On the other hand, the gap vanishes right at the critical point so the adiabaticity conditions can never be satisfied in the vicinity of the phase transition. The slower the parameter changes the more time the system spends near the critical point, but on the other hand the less the interval where the adiabaticity is violated. The competition between these two processes determines the total amount of excitations in the system. Here, we show that the number of excited states decreases as a power law of the tuning rate. Because of the universality and scaling, below a certain dimension, which we identify later, this power is determined by the critical exponents z and ν characterizing the transition. So measuring the number of excitations as a function of the tuning rate one can obtain the information about the critical properties of the phase transition. We give a general argument for the particular scaling form and consider two specific examples of phase transitions occurring within Boson Hubbard- and transverse field Ising models, which confirm this scaling.

Let us start from a general formalism. We assume that the system is described by some Hamiltonian $\mathcal{H}(\lambda)$, which depends on the external parameter λ. Without loss of generality $\lambda=0$ corresponds to the phase boundary, so that $\lambda>0$ and $\lambda<0$ describe different phases of the system. Let the set of (many-body) functions $\phi_r(\lambda)$ represent the eigenbasis of the Hamiltonian $\mathcal{H}$. The wave function of the system can be always expanded in this basis:

$$\psi=\sum_p a_p(t)\phi_p(\lambda). \quad (1)$$

We assume that λ slowly changes in time: $\lambda(t)=\delta t$, where δ is the adiabaticity parameter and we took linear dependence on time for the sake of convenience. Then, substituting Eq. (1) into Schrödinger equation, we find:

$$i\frac{da_p}{dt}+i\delta\sum_q a_q(t)\langle p|\frac{d}{d\lambda}|q\rangle=\omega_p(\lambda)a_p(t), \quad (2)$$

where $\omega_p(\lambda)$ is the eigenfrequency of the Hamiltonian $\mathcal{H}(\lambda)$. It is convenient to perform a unitary transformation:

$$a_p(t)=\tilde{a}_p(t)e^{-i\int^t\omega_p(\lambda(t))dt}=\tilde{a}_p(\lambda)e^{-i/\delta\int^\lambda\omega_p(\lambda)d\lambda}. \quad (3)$$

Combining Eqs. (2) and (3), we derive:

$$\frac{d\tilde{a}_p}{d\lambda}=-\sum_q\tilde{a}_q(\lambda)\langle p|\frac{d}{d\lambda}|q\rangle e^{i/\delta\int^\lambda(\omega_p(\lambda')-\omega_q(\lambda'))d\lambda'}. \quad (4)$$

If before the evolution the system was in the ground state $|0\rangle$ then a single term dominates the sum in Eq. (4). The relative number of the excited states is thus given by

$$n_{\mathrm{ex}}\approx\sum_p{}' \left|\int_{-\infty}^{\infty}d\lambda\langle p|\frac{d}{d\lambda}|0\rangle e^{i/\delta\int^\lambda(\omega_p(\lambda')-\omega_0(\lambda'))d\lambda'}\right|^2, \quad (5)$$

where the prime over the sum implies that the summation is taken only over the excited states. It is important to emphasize that across the second-order phase transition, which we consider in this paper, the basis wave functions change continuously with λ.

Let us assume that we deal with a uniform d-dimensional system. This assumption is not necessary, but it is the case for the most known systems undergoing a quantum phase transition. We also assume that there is a single branch of excitations characterized by the gap Δ and some dispersion. Since both Δ and λ become zero at the phase boundary then, near the critical point, we must have $\Delta \propto |\lambda|^{z\nu}$ [1] with z and ν being critical exponents. In the momentum space (5) reduces to:

$$n_{\rm ex} \approx \int \frac{d^dk}{(2\pi)^d} \left| \int_{-\infty}^{\infty} d\lambda \langle k|\frac{d}{d\lambda}|0\rangle e^{i/\delta \int^{\lambda}(\omega_k(\lambda')-\omega_0(\lambda'))d\lambda'} \right|^2. \tag{6}$$

From general scaling arguments, we can write:

$$\omega_k - \omega_0 = \Delta F(\Delta/k^z) = \lambda^{z\nu}\widetilde{F}(\lambda^{z\nu}/k^z), \tag{7}$$

where $F(\widetilde{F})$ is some undefined function satisfying $F(x) \propto 1/x$ for large x, and z is the dynamic critical exponent. Similarly, we can argue that

$$\langle k|\frac{\partial}{\partial\Delta}|0\rangle = \frac{1}{k^z}G(\Delta/k^z) \Rightarrow \langle k|\frac{\partial}{\partial\lambda}|0\rangle = \frac{\lambda^{z\nu-1}}{k^z}\widetilde{G}(\lambda^{z\nu}/k^z), \tag{8}$$

where $G(\widetilde{G})$ is another scaling function satisfying $G(0)$ =const. Having these scaling forms in mind, we can do the following substitutions in Eq. (6): $\lambda = k^{1/\nu}\xi$, $k=\delta^{\nu/z\nu+1}\eta$. It is easy to see that if the momentum integral in Eq. (6) can be extended to infinity then:

$$n_{\rm ex} = C\delta^{d\nu/(z\nu+1)}, \tag{9}$$

where C is a nonuniversal constant which depends on the details of the transition. The condition allowing to send the upper cutoff to infinity is $d<d_c=2z(z\nu+1)$, where d_c is the upper critical dimension for this problem. Note that ν and z can depend on d themselves. For $d>d_c$, the main contribution to the excitations comes from the high momentum states. In this case, $n_{\rm ex}$ would still vanish at $\delta\to 0$, but the universality will disappear as excitations with high momenta ($k^z \gg \Delta$) will dominate the transitions. The result (9) is quite remarkable, it shows that if $\delta\to 0$ and ν is a finite number greater then zero, the transitions to the excited states are suppressed and the adiabatic limit still holds. We want to emphasize, the adiabaticity is understood in a sense that the density, not the total number, of excitations is much smaller than one. Strictly speaking in the true adiabatic limit, there should be no excitations and the system must remain in the ground state. However to achieve this, it is necessary to scale δ as inverse power of the system size,[5] which is virtually impossible to do in large systems. There are two limits $\nu\to 0$ and $\nu\to\infty$ in Eq. (9) which require special attention. The first one is trivial since it corresponds to the absence of the phase transition since the gap always remains finite except for a very narrow interval around $\lambda=0$. Indeed, a more careful analysis shows that the constant C in Eq. (9) is proportional to ν.[2] The opposite limit $\nu\to\infty$ is more interesting since it corresponds to, e.g., Kosterlits–Thouless (KT) transition,[6] which has many realizations in 1+1 dimensional quantum systems. Thus, if the precise scaling form is $\Delta \propto e^{-b/\lambda^r}$ then

$$n_{\rm ex} \propto \delta_z^{\frac{d}{z}} \ln^{(r+1)(d-2z)/rz}(\delta^{-1}). \tag{10}$$

This expression acquires extra logarithmic corrections as compared to (9). In particular, for the KT transition $r=1/2$ and $z=1$ so that Eq. (10) reduces to

$$n_{\rm ex}^{\rm KT} \propto \delta^d \ln^{3(d-2)}(\delta^{-1}). \tag{11}$$

There are no logarithmic corrections in two dimensions. However, the only physically relevant case where the KT transition can occur in a quantum system at zero temperature corresponds to $d=1$.

Qualitatively, one can interpret Eq. (9) in a simple way. The transitions to the excited states occur when the adiabaticity conditions break down, i.e., when $d\ln\Delta/dt \gg \Delta$. From this, one immediately finds that the time interval when the transitions take place scales as: $t\sim\delta^{-z\nu/z\nu+1}$. The typical gap at this time scale is

$$\Delta \sim (\delta t)^{z\nu} \sim \delta^{z\nu/z\nu+1}, \tag{12}$$

which amounts to the available phase space $\Omega\sim k^d\sim\Delta^{d/z} \sim \delta^{d\nu/z\nu+1}$. Now, if we use the anzats that $d\Delta\langle k|\partial/\partial\Delta|0\rangle$ is a scale independent quantity [see Eq. (8)], then we immediately come to the conclusion that this phase space determines the number of excited states $n_{\rm ex}$ so that we come to Eq. (9). This simple derivation above, in fact, does not rely on the spatial homogeneity of the system. The only information we need is the density of states of excitations $\rho(\epsilon)$ at the energy scale determined by Eq. (12). So, in a general case instead of Eq. (9), we get:

$$n_{\rm ex} \propto \delta^{z\nu/z\nu+1}\rho(\delta^{z\nu/z\nu+1}). \tag{13}$$

Notice that Eq. (9) contains only two critical exponents ν and z. So measuring the dependence $n_{\rm ex}(\delta)$ and knowing one of the exponents, say z, one can immediately deduce other.

Let us apply these ideas to the superfluid-to-insulator transition in a system of interacting bosons in a d-dimensional lattice at commensurate filling.[1,7] To describe the excitations near the critical point, we adopt a mean-field Hamiltonian derived by Altman and Auerbach in Refs. 8 and 9:

$$\begin{aligned}\mathcal{H} = 2dJN\sum_{\mathbf{k}} \Bigg\{ &(2u\cos\theta - \cos 2\theta + \epsilon_{\mathbf{k}}\cos^2\theta) b_{1,\mathbf{k}}^\dagger b_{1,\mathbf{k}} \\ &- \frac{1-\epsilon_{\mathbf{k}}}{2}\cos^2\theta(b_{1,\mathbf{k}}^\dagger b_{1,-\mathbf{k}}^\dagger + b_{1,\mathbf{k}}b_{1,-\mathbf{k}}) \\ &+ \left(2u\cos^2\frac{\theta}{2} + \sin^2\theta - \cos^2\frac{\theta}{2} + \epsilon_{\mathbf{k}}\cos^2\frac{\theta}{2}\right) b_{2,\mathbf{k}}^\dagger b_{2,\mathbf{k}} \\ &+ \frac{1-\epsilon_{\mathbf{k}}}{2}\cos^2\frac{\theta}{2}(b_{2,\mathbf{k}}^\dagger b_{2,-\mathbf{k}}^\dagger + b_{2,\mathbf{k}}b_{2,-\mathbf{k}}) \Bigg\}. \end{aligned} \tag{14}$$

Here, J is the tunneling constant, N is the mean number of bosons per site, which we assume to be a large integer for the sake of simplicity, $\epsilon_{\mathbf{k}} = 1/2d\Sigma_\delta 1 - e^{i\mathbf{k}\delta}$, θ is the mean field angle characterizing the phase. In particular $\theta=0$ corresponds to the Mott phase, while in the superfluid regime $\cos\theta \approx u$. The dimensionless interaction $u \equiv U/(4JdN)$ is defined so that the transition occurs at $u=1$.

In the Mott side of the transition, $u>1$, both branches are degenerate and the Hamiltonian (14) can be readily diagonalized via the Bogoliubov's transformation:

$$\beta_{m,\mathbf{k}} = \cosh\phi_{m,\mathbf{k}} b_{m,\mathbf{k}} - \sinh\phi_{m,\mathbf{k}} b^\dagger_{m,-\mathbf{k}}, \tag{15}$$

where it becomes

$$\mathcal{H} = \sum_{m,\mathbf{k}} \omega_{m,\mathbf{k}} \beta^\dagger_{m,\mathbf{k}} \beta_{m,\mathbf{k}}. \tag{16}$$

The eigenfrequencies $\omega_{m,\mathbf{k}}$ and the angle $\phi_{m,\mathbf{k}}$ read:

$$\omega_{1,2,\mathbf{k}} = 4dJNu\sqrt{\frac{u-1}{u} + \frac{\epsilon_\mathbf{k}}{u}} \approx 4dJN\sqrt{\lambda + \epsilon_\mathbf{k}}, \tag{17}$$

$$\tanh 2\phi_{1,2,\mathbf{k}} = \pm \frac{1-\epsilon_\mathbf{k}}{2\lambda + 1 + \epsilon_\mathbf{k}}, \tag{18}$$

We have chosen $\lambda = u-1$ to be the parameter governing the phase transition. Given Hamiltonian (16) and transformations (15) it is easy to write down the ground-state wave function:

$$|0\rangle = \prod_{m,\mathbf{k}} \cosh\phi_{m,\mathbf{k}} e^{\tanh\phi_{m,\mathbf{k}} b^\dagger_{m,\mathbf{k}} b^\dagger_{m,-\mathbf{k}}} |Vac\rangle, \tag{19}$$

where $|Vac\rangle$ is the state with no b particles. It is a simple exercise to check that $\langle p|\partial/\partial\lambda|0\rangle$ is non zero only when two particles with opposite momenta are excited, i.e.,

$$|p\rangle \equiv |m,\mathbf{k},-\mathbf{k}\rangle = b^\dagger_{m,\mathbf{k}} b^\dagger_{m,-\mathbf{k}}|0\rangle. \tag{20}$$

Then, it can be verified that

$$\langle m,\mathbf{k},-\mathbf{k}|\frac{\partial}{\partial\lambda}|0\rangle = \mp\frac{1}{2}\frac{1-\epsilon_\mathbf{k}}{(1+\lambda)(\lambda+\epsilon_\mathbf{k})} \approx \mp\frac{1}{2(\lambda+\epsilon_\mathbf{k})}, \tag{21}$$

where we used the approximation that both λ and $\epsilon_\mathbf{k}$ are small near the phase transition. Note that Eq. (21) satisfies the general scaling (8) with the exponent $\nu=1/2$, in the same way the dispersion relation (17) agrees with Eq. (7).

A similar analysis can be performed on the superfluid side. The Hamiltonian (14) now gives two branches corresponding to the amplitude and the phase modes:

$$\omega_{1,\mathbf{k}} \approx 4dJN\sqrt{-\lambda + \epsilon_\mathbf{k}}, \quad \omega_{2,\mathbf{k}} \approx 4dJN\sqrt{\epsilon_\mathbf{k}}, \tag{22}$$

which are characterized by the following angles of the transformation (15):

$$\tanh 2\phi_{1,\mathbf{k}} \approx \frac{1-\epsilon_\mathbf{k}+2\lambda}{1+\epsilon_\mathbf{k}}, \quad \tanh 2\phi_{2,\mathbf{k}} \approx \frac{2-2\epsilon_\mathbf{k}+\lambda}{2+2\epsilon_\mathbf{k}+\lambda}. \tag{23}$$

Note that the parameter λ is negative on the superfluid side. The matrix elements for these two modes are:

$$\langle 1,\mathbf{k},-\mathbf{k}|\frac{\partial}{\partial\lambda}|0\rangle \approx -\frac{1}{2(\epsilon_\mathbf{k}-\lambda)}, \quad \langle 2,\mathbf{k},-\mathbf{k}|\frac{\partial}{\partial\lambda}|0\rangle \approx \frac{1}{4}. \tag{24}$$

The excitations of the phase modes are suppressed as compared to the amplitude ones. This can be also expected on the physical grounds, i.e., by changing the parameter λ or equivalently u we change the mass or the gap of the amplitude mode thus exciting it, however, there is no such a coupling mechanism for the phase mode. Clearly, the total number of the excited phase oscillations is not determined by the properties of the critical point and thus is not universal. This number scales as $n_{\mathrm{ex}} \propto \delta^d$, i.e., vanishes much faster with δ than the number of excitations to the gapped mode. Besides, a typical experiment would use the phase contrast as a measure of superfluidity,[3,10] which is not strongly affected by low momentum phase excitations. Keeping this in mind, we calculate explicitly only the number of particle pairs lost to the mode 1, which is gapped on both sides of the transition. Experimentally, this number can be detected by getting first from the superfluid to the Mott insulator and then returning back to the superfluid regime and measuring the loss of the phase contrast, or by measuring the number of created particle-hole pairs in the insulating state. Performing the integration in Eq. (6) we find that in one, two, and three dimensions, the number of excitations is

$$n_{\mathrm{ex}}^{1\mathrm{D}} \approx 0.348\left(\frac{\delta}{JN}\right)^{1/3}, \quad n_{\mathrm{ex}}^{2\mathrm{D}} \approx 0.059\left(\frac{\delta}{JN}\right)^{2/3},$$

$$n_{\mathrm{ex}}^{3\mathrm{D}} \approx 0.010\left(\frac{\delta}{JN}\right), \tag{25}$$

respectively. We note that since $\nu=1/2$ within this meanfield treatment and $z=1$, the upper critical dimension is $2z(z\nu+1)=3$ so the scaling (9) is valid in one and two dimensions. However, this model has an additional symmetry, giving the same prefactors of the gap and wave function dependence on λ in both superfluid and insulating phases [compare Eq. (17) with Eqs. (22) and (21) with (24)]. This symmetry shifts the upper critical dimension to $d=4$, so the results remain universal in all three spatial dimensions. As anticipated, expressions (25) are consistent with Eq. (9).

The correct description of the superfluid-to-insulator transition gives exponents different from the mean-field values used above. The commensurate transition lies in the universality class of the XY model in the $d+1$ dimensions with $z=1$ and $\nu=0.5$ for $d=3$, $\nu\approx 0.67$ for $d=2$,[11] and $\nu=\infty$ in $d=1$ (Ref. 6) [more precisely, the universality class in the latter case is of the KT transition with $\Delta \propto \exp(-b/\sqrt{\lambda})$]. So that for these special points Eq. (9) reduces to

$$n_{\mathrm{ex}}^{1\mathrm{D}} \propto \frac{\delta}{\ln^3(\delta^{-1})}, \quad n_{\mathrm{ex}}^{2\mathrm{D}} \propto \delta^{0.80}, \quad n_{\mathrm{ex}}^{3\mathrm{D}} \propto \delta. \tag{26}$$

In a generic point of the superfluid-insulator transition corresponding to the noncommensurate filling $z\nu=1$[7] and since $z\geqslant 1$, the upper critical dimension d_c is always larger than 3. So Eq. (9) reduces to: $n_{\mathrm{ex}} \propto \delta^{d/2\nu}$. Thus measuring $n_{\mathrm{ex}}(\delta)$, it is possible to observe the exponent ν. Unfortunately except for $3D$, where $\nu=1/2$ and hence $n_{\rm ex}\propto\delta^{3/4}$, the precise value of ν (and z) is not fixed but rather depends on the point where the transition occurs.[12]

Another example we consider here is the transverse field Ising model,[1] which is described by the Hamiltonian

$$\mathcal{H}_I=-\sum_j g\sigma_j^x+\sigma_j^z\sigma_{j+1}^z, \tag{27}$$

where σ_x and σ_z are the Pauli matrices. The dimensionless coupling constant g drives the system through a critical point, which occurs at $g_c=1$ (Ref. 1) and which is characterized by the critical exponents $z=\nu=1$. Using the Jordan–Wigner transformation, one can show that Eq. (27) maps to the model of free spinless fermions with the Hamiltonian

$$\mathcal{H}_I=-\sum_j c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j+c_j^\dagger c_{j+1}^\dagger+c_{j+1}c_j-2gc_j^\dagger c_j, \tag{28}$$

which in turn can be diagonalized by the Bogoliubov's transformation:

$$c_k=\cos(\theta_k/2)\gamma_k+i\sin(\theta_k/2)\gamma_{-k}^\dagger. \tag{29}$$

Here, c_k is the Fourier transform of c_j and the angle θ_k is given by[1]

$$\tan\theta_k=\frac{\sin(ka)}{\cos(ka)-g}. \tag{30}$$

In the diagonal form, the Hamiltonian (28) reads

$$\mathcal{H}_I=\sum_k\varepsilon_k\gamma_k^\dagger\gamma_k, \tag{31}$$

where $\varepsilon_k=2\sqrt{1+g^2-2g\cos k}$. The ground-state wave function, which is the vacuum of Eq. (31) reads

$$|\Omega\rangle=\prod_k[\cos(\theta_k/2)+i\sin(\theta_k/2)c_k^\dagger c_{-k}^\dagger]|0\rangle, \tag{32}$$

where $|0\rangle$ is the state with no c-fermions. The excited states have the form of $\gamma_{k1}^\dagger\gamma_{k2}^\dagger\ldots\gamma_{kn}^\dagger|\Omega\rangle$. The natural choice of the tuning parameter λ is $\lambda=g-1$ which is proportional to the energy gap Δ. It is straightforward to verify that

$$\frac{\partial}{\partial\lambda}|\Omega\rangle=\frac{i}{2}\sum_k\frac{\partial\theta_k}{\partial g}\gamma_k^\dagger\gamma_{-k}^\dagger|\Omega\rangle=\frac{i}{2}\sum_k\frac{\sin k}{1+g^2-2g\cos k}\gamma_k^\dagger\gamma_{-k}^\dagger|\Omega\rangle, \tag{33}$$

which again corresponds to two particle excitations. This expression is consistent with Eq. (8) with $G(0)=i/2$. Now using Eq. (6), we immediately find:

$$n_{\rm ex}\approx 0.18\sqrt{\delta}, \tag{34}$$

which agrees with the general formula (9) given that $d=\nu=z=1$.

In conclusion, we showed that if the system, originally in the ground state, is slowly driven through a quantum critical point, the number of excited states per unit volume goes to zero as a power law of the tuning rate. The exponent is universal and is determined by the critical properties of the transition if the dimension is smaller then $d_{\rm cr}=2z(z\nu+1)$. We provided some general arguments and performed explicit calculations for the superfluid-to-insulator transition within the Boson Hubbard model and for the quantum phase transition in the transverse field Ising model.

Recently, two other papers appeared, which addressed a similar issue of the number of created defects for a specific case of a transverse field Ising model.[13,14] In particular, the authors got the same scaling as in Eq. (34) but with a slightly smaller numerical prefactor. The discrepancy comes from a more accurate treatment of transition probabilities within the Landau–Zener formalism.[15]

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